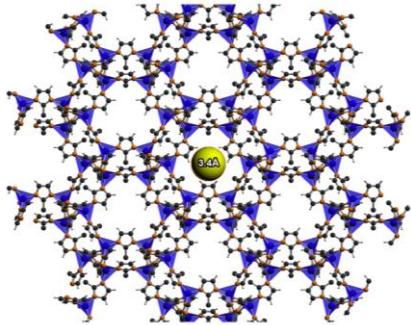


Nanoporous Mixed-Matrix Membranes for Gas Separations

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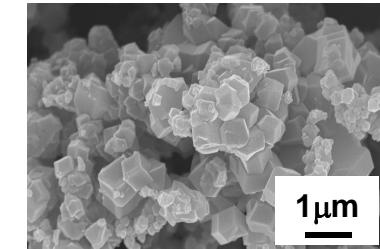
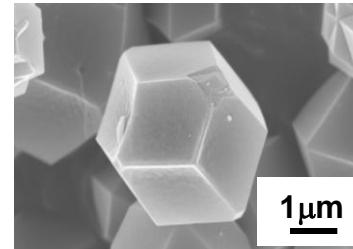
ZIF-8, ZIF-20, ZIF-69, ZIF-95, and ZIF-100 are candidates for CO₂ capture

e.g.
ZIF-8

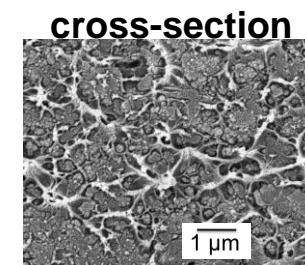
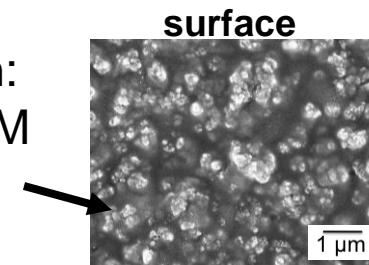


Synthesis:

- Hydrothermal
- microwave



Membrane formation:
ZIF-8/Matrimid® MMM
e.g. 50% composition



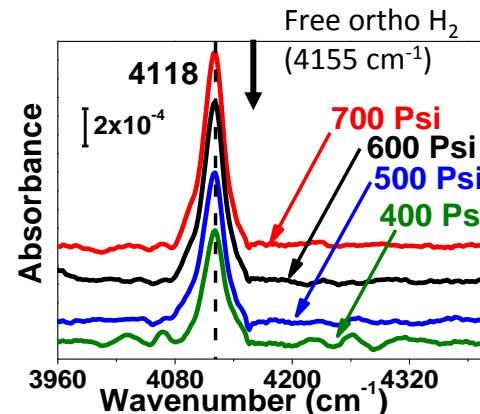
Permeability and Selectivity better for pure polymer matrix, e.g. $\alpha(\text{CO}_2/\text{CH}_4) > 150$

Fundamental understanding and control of Interaction of guest molecules with MOF

In-situ IR absorption measurements:

- Room temp., high pressures (20-60 bars)
- Low temp. (4-100K) and P (.01-.5 bar)

$$\Delta\nu(\text{H-H}) \sim -37 \text{ cm}^{-1}$$



Novel van der Waals-Density Functional theory

(Troullier-Martins pseudo-potentials + gradient correction)

→ interaction energies and frequency shifts calculated within 0.1 kJ/mol and 1 cm⁻¹.

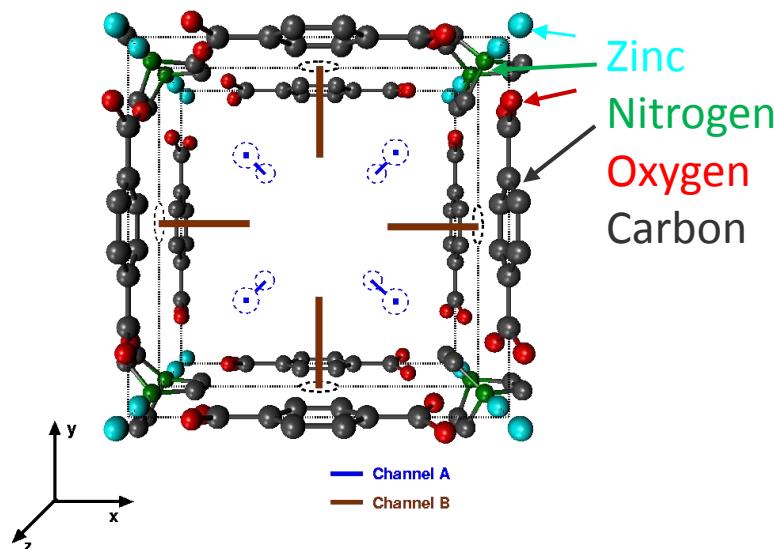
Calculated H₂ binding energy

~ 10 KJ/mole

- E_{zero point} ~ 3 KJ/mole

= 7 KJ/mole

Calculated $\Delta\nu(\text{H-H}) \sim -30\text{-}32 \text{ cm}^{-1}$



Experimental and theoretical tools in place to derive location and interaction energies for a variety of guest molecules in MOF → guide to design MOF to optimize gas separation